

Ternary configuration in the framework of inverse mean-field method

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Abstract. A static scission configuration in cold ternary fission has been considered in the framework of mean field approach. The inverse scattering method is applied to solve single-particle Schrödinger equation, instead of constrained selfconsistent Hartree–Fock equations. It is shown, that it is possible to simulate one-dimensional three-center system via inverse scattering method in the approximation of reflectless single-particle potentials.

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1. Introduction

Ternary fission involving the emission of α -particle was first observed [1] more than fifty years ago. Emission of α -particles in the spontaneous fission of ^{252}Cf has also a long history of investigation experimentally [2] and theoretically [3, 4].

A renewed interest in the spontaneous fission of ^{252}Cf arose in connection with modern experimental techniques, $\gamma - \gamma - \gamma$ and $x - \gamma - \gamma$ triple coincidence, (Gammasphere with 110 Compton suppressed Ge detectors), which allow the fine resolution of the mass, charge and angular momentum content of the fragments[5]. Very recently direct experimental evidence was presented for the cold (neutronless) ternary spontaneous fission of ^{252}Cf in which the third particle is an α -particle [6], or ^{10}Be [7]. This confirms that a large variety of nuclear large-amplitude collective motions such as bimodal fission [8], cold binary fission [5, 9, 10, 11, 12], heavy cluster radioactivity [14, 13], and inverse processes, such as subbarrier fusion [15], could belong to the general phenomenon of cold nuclear fragmentation.

The main common characteristic of cold binary nuclear fragmentation is the emission of the final fragments (nuclei) with very low or even zero excitation energy and consequently with high total kinetic energy (TKE), which can be provided only with compact shapes of fragments at the scission point [16, 17]. The cold ternary fragmentations should also have compact shapes at scission with deformations close to those of their ground states, in order to achieve high TKE values tending to the ternary decay energy Q_t . It is assumed, that a light nucleus (e.g. an alpha-particle, Be etc.) is formed at the surface of the initial nucleus, and that the two heavier fragments are formed at the scission configuration in their ground states.

These cluster like models [16, 17] were used successfully to reproduce general features of the cold ternary fragmentation. However the scission configuration has been built in fact by hands. Therefore it is actual to develop microscopical or semi-microscopical approach to this scission-point concept of nuclear fragmentation.

Recent experimental progress in the production of superheavy elements [18] near the proposed superheavy "island of stability" [19] has stimulated yet the critical reexamination of earlier extrapolations [20, 21, 22, 23] of the nuclear shell structure. Although this macroscopic-microscopic models quite successfully describe the bulk properties of known nuclei, their parameterization needs preconceived knowledge about the density distribution and the nuclear potentials which fades away when going to the limits of stability. Therefore it is actual to investigate the properties of superheavy elements with self-consistent models, like the mean-field models based on the shell correction method, self-consistent Skyrme-Hartree-Fock (SHF) [24] and relativistic mean-field (RMF) models (see [29, 25, 26, 27, 28] and refs. therein).

There are well developed methods to calculate, in the framework of many-body self-consistent approach, static properties of a well isolated nucleus in its ground state. There also exists a well developed two-center shell model [30]. However, a three-center shell model has not been developed yet, except for very early steps [31]. Three-center shapes

are practically not investigated, in comparison with the two-center ones. There exists the generalizations of mean-field models to the case of two-centers [32], but a ternary configuration is out of consideration, because of uncertainties to select a peculiar set of constraints.

There also exist a number of calculations for nucleus-nucleus collisions in the frame of time-dependent mean-field methods, but an evolution of the cold fragmentation has not been investigated yet.

Therefore, although the principal way to describe nuclear fragmentation in the framework of many-body self-consistent approach exists, it is interesting to develop other mean-field approaches to analyse these phenomena from different points of view.

We suggest to use the methods of nonlinear dynamics. These methods gave yet the possibility to derive for nuclear physics unexpected collective modes, which can not be obtained by traditional methods of perturbation theory near some equilibrium state (see [33, 34, 35, 36, 37] for the recent refs.). The most important reason is that the fragmentation and clusterization is a very general phenomenon. There are cluster objects in subnuclear and macro physics. Very different theoretical methods were developed in these fields. However, there are only few basic physical ideas, and most of the methods deal with nonlinear partial differential equations. One of the most important part of soliton theory is the inverse scattering method [38, 39, 40] and its applications to the integration of nonlinear partial differential equations [41].

In this Letter, we simulate three-center configuration using inverse scattering method to solve the single-particle Schroedinger equation, instead of direct solution of constrained Hartree-Fock equations.

2. The framework

The inverse methods to integrate nonlinear evolution equations are often more effective than a direct numerical integration. Let us demonstrate this statement for the following simple case. The type of systems under consideration are slabs of nuclear matter [42], which are finite in the z coordinate and infinite and homogeneous in two transverse directions. The wave function for the slab geometry is

$$\psi_{\mathbf{k}_\perp n}(\mathbf{x}) = \frac{1}{\sqrt{\Omega}} \psi_n(z) \exp(i\mathbf{k}_\perp \mathbf{r}), \quad \epsilon_{\mathbf{k}_\perp n} = \frac{\hbar^2 k_\perp^2}{2m} + e_n, \quad (1)$$

where $\mathbf{r} \equiv (x, y)$, $\mathbf{k}_\perp \equiv (k_x, k_y)$, and Ω is the transverse normalization area.

$$-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} \psi_n(z) + U(z) \psi_n(z) = e_n \psi_n(z), \quad (2)$$

A direct method to solve the single-particle problem (2) is to assign a functional of interaction \mathcal{E} (usually an effective density dependent Skyrme force), to derive the ansatz for the one-body potential, as the first variation of a functional of interaction in density $U(z) = U[\rho(z)] = \delta\mathcal{E}/\delta\rho$. Then to solve the Hartree-Fock problem under the set of constraints, which define the specifics of the nuclear system. In the simplest case of a

ground state, one should conserve the total particle number of nucleons (A), which is related to the "thickness" of a slab, via $A \Rightarrow \mathcal{A} = (6A\rho_N^2/\pi)^{1/3}$, which gives the same radius for a three-dimensional system and its one-dimensional analogue. As a result, one obtains the energies of the single particle states e_n , their wave functions $\psi_n(z)$, the density profile $\rho(\mathbf{x}) \Rightarrow \rho(z)$

$$\rho(z) = \sum_{n=1}^{N_0} a_n \psi_n^2(z), \quad \mathcal{A} = \sum_{n=1}^{N_0} a_n, \quad a_n = \frac{2m}{\pi\hbar^2}(e_F - e_n), \quad (3)$$

and the corresponding single-particle potential. a_n are the occupation numbers, N_0 is the number of occupied bound orbitals. The Fermi-energy e_F controls the conservation of the total number of nucleons. The energy (per nucleon) of a system is given by

$$\frac{E}{A} \Rightarrow \frac{\hbar^2}{2m\mathcal{A}} \left(\sum_{n=1}^{N_0} a_n \int_{-\infty}^{\infty} \left(\frac{d\psi_n}{dz} \right)^2 dz + \frac{\pi}{2} \sum_{n=1}^{N_0} a_n^2 \right) + \frac{1}{\mathcal{A}} \int_{-\infty}^{\infty} \mathcal{E}[\rho(z)] dz. \quad (4)$$

Finally, the set of formulas (1–4) completely defines the direct self-consistent problem. Following the inverse scattering method, one reduces the main differential Schrödinger equation (2) to the integral Gel'fand-Levitan-Marchenko equation [38, 39]

$$K(x, y) + B(x + y) + \int_x^{\infty} B(y + z) K(x, z) dz = 0. \quad (5)$$

for a function $K(x, y)$. The kernel B is determined by the reflection coefficients $R(k)(e_k = \hbar^2 k^2 / 2m)$, and by the N bound state eigenvalues

$$B(z) = \sum_{n=1}^N C_n^2(\kappa_n) + \frac{1}{\pi} \int_{-\infty}^{\infty} R(k) \exp(ikz) dk, \quad e_n = -\hbar^2 \kappa_n^2 / 2m.$$

N is the total number of the bound orbitals. The coefficients C_n are uniquely specified by the boundary conditions and the symmetry of the problem under consideration. The general solution, $U(z) = -(\hbar^2/m)(\partial K(z, z)/\partial z)$, should naturally contain both, contributions due to the continuum of the spectrum and to its discrete part. There seems to be no way to obtain the general solution $U(z)$ in a closed form. Eqs. (2),(5) have to be solved only numerically. In Ref. [43] we used the approximation of reflectless ($R(k) = 0$), symmetrical ($U(-z) = U(z)$) potentials. This gave the possibility to derive the following set of relations

$$\begin{aligned} U(z) &= -\frac{\hbar^2}{m} \frac{\partial^2}{\partial z^2} \ln(\det \|M\|) = -\frac{2\hbar^2}{m} \sum_{n=1}^N \kappa_n \psi_n^2(z), \\ \psi_n(z) &= \sum_{l=1}^N (M^{-1})_{nl} \lambda_l(z), \quad \lambda_n(z) = C_n(\kappa_n) \exp(-\kappa_n z), \\ M_{nl}(z) &= \delta_{nl} + \frac{\lambda_n(z) \lambda_l(z)}{\kappa_n + \kappa_l}, \quad C_n(\kappa_n) = \left(2\kappa_n \left| \prod_{l \neq n}^N \frac{\kappa_n + \kappa_l}{\kappa_n - \kappa_l} \right| \right)^{1/2}. \end{aligned} \quad (6)$$

Consequently, in the approximation of reflectless potentials ($R(k) = 0$), the wave functions, the single-particle potential and the density profiles are completely defined by the bound state eigenvalues via formulas (1),(6).

3. Results and Discussion

In Ref. [43] a series of calculations for the different layers, imitating nuclear systems in their ground state was provided. For a direct part of the calculations by the Hartree-Fock method, the interaction functional was chosen in the form of effective Skyrme forces. The calculated spectrum of bound states was fed into the scheme of the inverse scattering method, and the relations were used to recover the wave functions of the states, the single-particle potentials, and the corresponding densities. In this note, we generalize this method to the case of fragmented configuration, trying to imitate two- and three-center nuclear systems. We use here only the inverse mean-field scheme (6). The details of the approach and systematic calculations of fragmented nuclear systems will be provided in a forthcoming publication. In Fig.1 we present the results of the

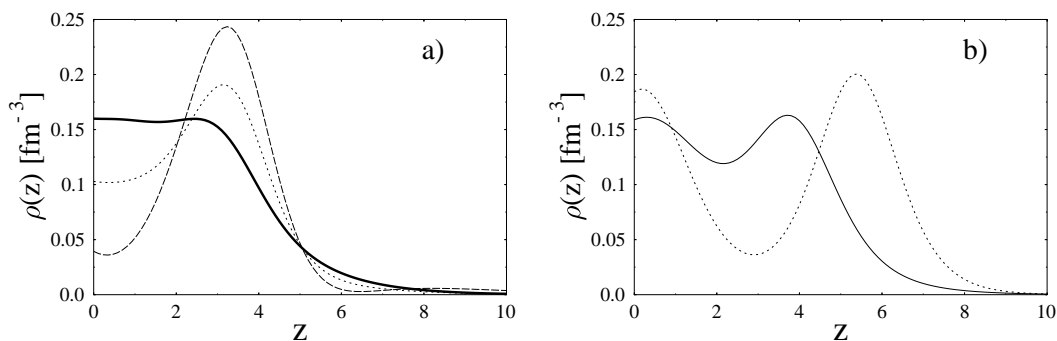


Figure 1. The density profiles of the light ($A \approx 20$, $\mathcal{A} \approx 1.0$) three-levels ($N = 3$, $N_0 = 3$) model system calculated in the frame of inverse mean field method. a) the ground state (solid line); a fragmented two-center configuration (dotted and dashed lines); b) a ternary fragmentation of the system into three fragments.

calculations of three-level ($N = 3$, $N_0 = 3$) light ($A \approx 20$, $\mathcal{A} \approx 1.0$) model system simulating the ground state (Fig. 1(a) solid line), and fragmentation of the system into two fragments (Fig. 1(a), the dotted and dashed lines). In the same figure (Fig. 1(b)) we present the fragmentation of the system into three fragments (solid and dotted lines). One can see that it is possible to simulate a one-dimensional three-center system via inverse scattering method. The following conclusions can be drawn.

- The density profiles, calculated in the framework of inverse method, are practically identical to the results of calculation by SHF method. These results are valid for the ground state and for the system in the external potential field.
- The global properties of single-particle potentials (the depth and an effective radius) have been reproduced quite well, but the inverse method yields the quite strongly pronounced oscillations of the potential distributions within the inner region, and slightly different asymptotic tails of potential. In the framework of inverse scattering method, all bound states are taken into account in the calculation of the potential (6), but for the density distribution only the occupied states are taken into account

(see Eqs. (3)). Therefore, the slope of the tails of the potential and of the density distributions will be different.

- We used, the approximation of reflectionless potentials, which gave us the possibility to obtain a simple closed set of relations (6), to calculate wave functions, density distributions and single particle potentials. The omitted reflection terms ($R(k) = 0$) are not important for the evaluation of the density distributions, due to the fact that only the deepest occupied states are used to evaluate density distribution (see Eq. (3)). The introduction of these reflection terms will lead to a smoothing of the oscillations in the inner part of the potential and to a correction of its asymptotic behaviour.
- The presented method gives a tool to simulate the various sets of the static excited states of the system. This method could be useful to prepare in a simple way an initial state for the dynamical calculations in the frame of mean-field methods.

4. Conclusions

Recent experimental progress in the investigation of cold nuclear fragmentation has made the development of theoretical many-body methods highly desirable. Modern variants of self-consistent Hartree-Fock and relativistic mean-field models give the principal way to describe nuclear fragmentation in the framework of many-body self-consistent approach. However, the generalization of these approaches to three-center case is not provided yet because of existing difficulties to select a suitable set of constraints.

We applied the inverse scattering method to solve the single-particle Schrödinger equation, instead of direct solution of constrained self-consistent Hartree-Fock equations. It is shown, that it is possible to simulate the one-dimensional three-center system via inverse scattering method.

It is needless to say that the present one-dimensional model is too primitive to describe a real three-dimensional fragmentation in nuclear systems. However this model may be useful as a guide to understand the general properties of fragmented systems and to formulate the suitable set of constraints for the realistic three-dimensional mean field calculations of the three-center nuclear system.

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